

4-Amino-1-naphthalenesulfonic acid sodium salt
130-13-2 | DTXSID0059611

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 192 °C

Global applicability domain: Inside

Local applicability domain index: 4.18e-01

Confidence level: 4.58e-01

Nearest Neighbors from the Training Set

Image not found

2-Amino-1-naphthalenesulfonic acid

Measured: 180

Predicted: 187

Image not found

Benzenesulfonic acid, 4-(phenylamino)-

Measured: 206

Predicted: 196

Image not found

6-Hydroxynaphthalene-2-sulfonic acid

Measured: 125

Predicted: 128

Image not found

5-Quinolinesulfonic acid, 8-hydroxy-

Measured: 323

Predicted: 197

Image not found

Sulfabenz

Measured: 200

Predicted: 194